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**Self-assembly of binary space-tessellating compounds** MIHIR KHADILKAR, UMANG AGARWAL, FERNANDO ESCOBEDO, Cornell University — Self-assembly of polyhedral nanoparticles and their mixtures has been a topic of interest in both experimental and simulation studies due to its potential to help engineer novel materials. Hard-core mixtures that tessellate space are particularly interesting since they are expected to form entropy-driven high-pressure ordered structures. Using Monte Carlo simulations, we study three such binary tessellating mixtures; namely, cuboctahedra + octahedra (Mixture 1), octahedra + tetrahedra (Mixture 2), and truncated cubes + octahedra (Mixture 3). We see that upon gradual compression of the isotropic system, Mixtures 1 and 2 form a metastable, glassy disordered phase while Mixture 3 demixes into a disordered phase and an unusual 'semi-crystalline' phase where truncated cubes form a cubic lattice while the octahedra remain disordered occupying interstitial pockets. While our results identify some relations between properties of individual species and their mixtures, they also illustrate the potential of tessellating mixtures as designable materials that can lead to novel equilibrium phases or serve as entropic glass formers. Preliminary results on non-tessellating binary mixtures will also be briefly discussed to provide a broader context of the results for the tessellating cases.

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